A major purpose of the Technical Information Center is to provide the broadest dissemination possible of information contained in DOE's Research and Development Reports to business, industry, the academic community, and federal, state and local governments.

Although a small portion of this report is not reproducible, it is being made available to expedite the availability of information on the research discussed herein.

# 1

CONF-860599-5

LA-UR-86-3819



LA-UR--86-3819

DE87 002912

TITLE: LESSONS FROM THE PAST AND PROSPECTS FOR THE FUTURE?

AUTHOR(S): Gordon Baym

SUBMITTED TO: To be included in proceedings of the CNLS Sixth Annual Conference "Nonlinearities in Condensed Matter," held in Los Alamos, May 4-9, 1986.



Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

DISTRIBUTION OF THIS DOCUMENT

Lessons from the Past and Prospects for the Future?

Gordon Baym

Theoretical Division
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
and
Department of Physics
University of Illinois at Urbana-Champaign
1110 W. Green St.
Urbana, Illinois 61801

## 1. INTRODUCTION

I must first of all point out that I am here under somewhat false pretenses, being a truly linear physicist who has not done serious work on any of the problems discussed this week. In fact, when I was a graduate student of Julian Schwinger's, we were firmly taught that all soluble problems could be reduced to the harmonic oscillator, the quintessential linear problem. [Of course, he was very skilled at transforming all sorts of problems, such as the hydrogen atom and angular momentum, to the harmonic oscillator.] I will thus not treat the subject on a state-by-state basis, diving into the various controversies we have heard, but only give an incomplete "statistical" thermodynamic overview of the meeting, trying to convey my impressions of how the conference answered its implicit assignment: what are the lessons from the past and prospects for the future?

The first lesson learned from all the wonderful talks this week is the enormous progress that has been made in entering the world of real nonlinearities and their role in condensed matter physics. The subject of nonlinearity in condensed matter is vital and growing, and taking shape as a major subfield. One cannot help but be impressed by the wide range of people from very different disciplines that have come together this week, ranging from condensed matter theorists and experimentalists, chemists, real materials people, mathematicians, and even a few high-energy and nuclear types. Equally impressive has been the wide range of problems, systems and materials considered: from anisotropic magnetic compounds, electronic materials such as polyacetylene, PDA, and other polymers, heavy fermion compounds, ferroelectrics, spin glasses, quasicrystals, charge-density wave materials, quantum-Hall materials, and other structured materials, to biological materials such as rhodopsin and DNA, to artificial structures, including electrical circuits and quasicrystalline superconducting loop arrays, and finally to macroscopic quantum systems.

## 2. LESSONS FROM THE PAST AND PRESENT

What are the major lessons we, or at least I, have learned? One is clearly the recognition of the important role that simplified pictures have played as starting points for understanding realistic systems. In its first phase, from 1927-33, the quantum theory of solids was concerned with developing the most elementary and qualitative descriptions, e.g., the free electron model of metals by Pauli and Sommerfeld, the nature of energy bands in solids by Bloch, Peierls, and Wilson, the origin of positive Hall coefficients by Peierls, the quantum basis of the coupling of elementary magnetic moments in ferromagnets by Heisenberg, etc. Indeed, only after 1933, with the introduction of the Wigner-Seitz method, were solid-state physicists first able to confront quantitatively the quantum theory of condensed matter systems with experiment on real solids [1]. We have barely stepped over this threshhold now with the nonlinear systems discussed at this meeting.

More generally, advances in understanding strongly interacting systems have tended to use linear models as guides. Examples are Landau's theory of superfluid He and his

Fermi liquid theory; both these theories of strongly interacting systems begin with a decomposition of states into quasiparticle "elementary excitations" – the linearization – and then include interactions as tractable nonlinearities.

The problem now is that we are beginning to face intrinsically nonlinear strongly-coupled systems, such as spin glasses and those with a quantized Hall effect, for which the starting simplifications are less obvious. In highly-structured materials, especially ones with randomness, the nature of the states and spectra remains a difficult problem, e.g., the role of itinerant versus localized modes. How does one develop systematic approaches to solving such nonlinear problems? Here we must turn, as a guide to understanding these systems, to a wider variety of starting points including exactly soluble models, numerical simulations, and occasional inspired guesses, such as Laughlin's wave function for the fractionally-quantized Hall effect.

Historically, the Ising, Heisenberg and other lattice models, both classical and quantum, have provided great insight into ferromagnetism and other cooperative phenomena, as more recently have lattice gauge theories, and model theories with solitons, such as sine-Gordon, into intrinsically nonlinear systems. Important connections, as we have heard, are also now being made between nonlinear condensed matter systems and relativistic field theories, such as those between polyactylene and the Gross-Neveu model, and magnetic models and conformally invariant field theories. Controversy over the utility of soluble models does not seem to be past us. The questions raised this week on the usefulness for magnetic systems of the Bethe Ansatz versus the elementary excitation, or spin wave, picture were a strong echo of Bloch's immediate reaction to Bethe's paper containing his Ansatz, shortly after Bloch (and Slater) invented spin waves, and Bloch showed that they would destroy spontaneous magnetization in one and two dimensions. As Bloch wrote to Peierls from Copenhagen on 6 November 1931, "It appears to me that Bethe's tedious algebraic manipulation [Ixereien] is somewhat academic in character, in particular because it does not sufficiently discuss the neighborhood of the lowest eigenvalues. I believe that in this regime, however, my calculations are reasonable, since they neglect only the exclusion of spins on the same site and this cannot play a role in a very dilute spin gas." [2]

Heisenberg, incidentally, did not conceive of his model in any way as an exactly soluble toy; rather he felt that he was solving ferromagnetism as a natural extension of his work on spin alignment, via exchange, in the helium atom. Only some two years after he began his work on ferromagnetism did he appear to worry about the connection of his model with Ising's. As he wrote then (July 1928) to Pauli, "I'd like very much if Weyl could try this problem [the Heisenberg model]. I've completely given it up. The whole question seems important to me on account of the similarity between my model and Ising's. My present view is that Ising should have obtained ferromagnetism if he had assumed sufficiently many neighbors (perhaps $s \geq 8$)... . That Ising uses this ['wild spatial'] model as an argument against ferromagnetism seems to me an indication that he did not understand in perspective his own work." [3]

The approach to nonlinear systems by means of controlled numerical simulations in lattice models, as discussed often this week, is becoming a significant tool, especially with the advent of large computer flop rates enabling high statistics Monte Carlo calculations. Particularly, we are beginning to have available exact and informative studies of small systems, such as magnetic, and those with charge-density waves, and fractionally-quantized Hall effect.

Once simple models are understood it is necessary to face the problem of their relations to real systems. As several examples this week made clear – for instance, the failure of pure sine-Gordon models of magnetic systems to take into account out-of-plane degrees of freedom – one must avoid the temptation to stretch the physics to make it fit the secure models; rather, failure of the simple model is a signal that more interesting physics is waiting to be dealt with. Still unresolved is the development of a convergent approach to polyacetylene, reconciling the momentum space versus real space, or solid-state versus chemical points of view, the question of "correlation versus dimerization gaps." To what extent do these approaches account for all the relevant degrees of freedom? The arguments are reminiscent of the ancient controversy that arose in the theory of ferromagnetism of Heisenberg's Heitler-London method versus Bloch's tight-binding Bloch-wave approach. Slater finally brought the two points of view into harmony in his 1930 paper on "Cohesion in monovalent metals," [4] where he discusses "the relations of the methods of Heisenberg and of Bloch," and shows that, as different bases to build perturbation expansions on, "they are essentially equivalent in their results when properly handled."

A further lesson is the importance of dynamical studies, both experimental and theoretical, beyond thermodynamic ones. We have seen many examples of the crucial role of dynamical response in elucidating the properties of systems, e.g., quantum spin chains, charge density waves, polymers, random field systems, and non-equilibrium systems such as spin glasses, whose states, as in many real materials, depend on the past history; in the latter, for instance, dynamical studies may be only way to probe the transition line in magnetic field, temperature plane. Systematic studies of finite frequency properties should prove invaluable as well in heavy fermion systems, quantum Hall systems, and quasicrystals, where one is only beginning to pin down the states.

What is the relation of the dynamics of real systems to theorists' integrable systems? For example, dynamics of spin-chains, as we have seen, appear to deviate substantially from simple kink-antikink scattering in sine-Gordon models. How does one deal with dynamical systems with a large or infinite number of crucial degrees of freedom? A particular challenge for the theorists is to develop numerical simulation techniques for predicting dynamics. How can one use Monte Carlo methods to go beyond study of elementary lattice thermodynamics and low lying excitations, to calculate scattering vertices, transport coefficients, correlation functions, and further dynamical response?

Another recurring theme this week has been the role of defects and impurities – dirt physics. Here we should not heed Pauli's advice to Peierls in 1931, "I consider it harmful when younger physicists become accustomed to order-of-magnitude physics. The residual resistance is a dirt effect and one shouldn't wallow in dirt," or later, "One shouldn't work on semiconductors, that's a filthy mess (Schweinerei)...." [5]. What are the effects of defects and impurities, e.g., in magnetic chains on solitons and diffusive behavior, in single crystal polymers, in charge-density-wave dynamics, in pinning of discommensurations, in ferroelectrics, etc.? A closely related and recurrent question has been the role of noise, ranging from problems of small systems, charge density wave motion, spin glasses, pattern growth, etc., to large systems exhibiting quantum coherence and interference.

One important lesson we have not yet learned is how generally to recognize the "smoking guns" of nonlinearity. What behavior is truly nonlinear, as for example that seen in the solitons in magnetic chains and in 3He-A, and in the existence of spinless charge carriers in polyacetylene? How does one distinguish dirt effects from nonlinearities, if possible; impurity problems, as we learned in the Kondo effect and can expect to see in heavy fermion systems, can themselves become highly nonlinear.

## 3. PROSPECTS FOR THE FUTURE

Although it is difficult to predict the course of the field of nonlinearities in condensed matter in detail, its future prospects, as brought out as this meeting, certainly appear very bright. The field, in possession of both very good theoretical tools and experimental techniques, e.g., resonance, and fabrication methods, is clearly emerging as one of the forefront subjects in condensed matter physics. Improvements in experimental techniques are driving the development of more accurate theory than we have at present. In addition to its more predictable developments, the field has and should continue to yield fascinating surprises, such as the integer and fractionally-quantized Hall effects, and heavy fermion compounds - two as intriguing as any in physics.

It is an inexpensive area, in contrast to large scale physics, and very important, both for its intrinsic physics interest and its possible applications. Overall the field is leading to a new sophisticated level of material science, on many scales, macro, meso, micro: including artificial and fabricated structures, and study of intrinsically inhomogeneous systems. To mention two examples discussed, the development of organic electronic materials as excellent nonlinear optical materials, and the very novel uses of superconductivity, from networks of Josephson junctions, to testing of quantum coherence on large scales.

Lastly, one of the pleasures of being the final speaker is to be able to acknowledge the hard work of the organizers of the meeting; I know that I speak for all of us in thanking Alan Bishop, David Campbell, Pradeep Kumar, and Steve Trullinger for all their efforts in giving us the opportunity to be exposed to and participate in such a fine overview of the present state of nonlinearities in condensed matter. I would also like to express my thanks to Doug Scalapino for conversations which helped to shape this summary.

* Supported in part by NSF Grant DMR84-15063.

REFERENCES

1. L. Hoddeson, G. Baym, and M. Eckert: Rev. Mod. Phys., Jan 1987.
2. Letter privately communicated by Felix Bloch.
3. Heisenberg to Pauli, 31 July 1928, in A. Hermann, K. von Meyenn, and V. F. Weisskopf (eds.), Wolfgang Pauli. Scientific Correspondence with Bohr, Einstein, Heisenberg, a.o., V. I: 1919-29 (Springer, Berlin, Heidelberg 1979).
4. J. C. Slater: Phys. Rev. 35, 509 (1930).
5. Pauli to Peierls in Ann Arbor, 1 July 1931, Pauli to Peierls, 29 Sept. 1931, in K. von Meyenn, A. Hermann and V. F. Weisskopf (eds.), Wolfgang Pauli. Scientific Correspondence with Bohr, Einstein, Heisenberg, a. o., V. II: 1930-1939 (Springer, Berlin. Heidelberg 1985).